Dependence of elastic constant on symmetry

Elastic behaviour of crystals is described by the **elastic stiffness tensor**

$$C_{ijkl}$$

which relates stress to strain via Hooke's law:

$$\sigma_{ij} = C_{ijkl}\,\varepsilon_{kl}$$

where

- σ_{ij}= stress tensor (2nd rank),
- ϵ_{kl}= strain tensor (2nd rank),
- C_{ijkl} = stiffness tensor (4th rank).

In three dimensions, the indices i, j, k, l can take values 1, 2, or 3 (x, y, z). This implies that the tensor C_{ijkl} generally has 3^4 = 81 components.

General properties:

(1) Minor Symmetries:

- $Symmetry\ of\ Stress$: $\sigma_{ij} = \sigma_{ji}$ $(Torque\ balance)$

Since $\sigma_{ij} = \sigma_{ji}$, the indices i and j are interchangeable in Hooke's Law.

$$C_{ijkl} = C_{jikl}$$

Originally, (i, j) has 3 x 3 = 9 combinations:

11, 12, 13, 21, 22, 23, 31, 32, 33

Because 12=21, 13=31, 23=32, we only have 6 unique combinations:

11, 22, 33, 23, 13, 12

New Count: We have 6 independent choices for (i,j) and still 9 choices for (k,l).

Total: 6 x 9 = 54 constants.

- $Symmetry\ of\ Strain: \epsilon_{kl} = \epsilon_{lk} (Definition\ of\ strain).$

Strain ϵ_{kl} is defined by the gradient of displacement u:

$$\epsilon_{kl} = \frac{1}{2}\left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k}\right)$$

Since $\epsilon_{kl} = \epsilon_{lk}$, the indices k and l are interchangeable in the stiffness tensor.

$$C_{ijkl} = C_{ijlk}$$

New Count: We have 6 choices for the "stress side" (i,j) and 6 choices for the "strain side" (k,l).

Total: 6 x 6 = 36 constants.

$$C = \begin{pmatrix} C_{1111} & C_{1122} & C_{1133} & C_{1123} & C_{1113} & C_{1112} \\ C_{2211} & C_{2222} & C_{2233} & C_{2223} & C_{2213} & C_{2212} \\ C_{3311} & C_{3322} & C_{3333} & C_{3323} & C_{3313} & C_{3312} \\ C_{2311} & C_{2322} & C_{2333} & C_{2323} & C_{2313} & C_{2312} \\ C_{1311} & C_{1322} & C_{1333} & C_{1323} & C_{1313} & C_{1312} \\ C_{1311} & C_{1222} & C_{1233} & C_{1223} & C_{1213} & C_{1212} \end{pmatrix}$$

(2) Major Symmetry

$$C_{ijkl} = C_{klij}$$

These symmetries reduce the number of independent components from **81 → 21** in the most general triclinic case.

Reduction of Constants (Voigt Notation)

These constraints reduce the number of independent constants from 81 to 21. To make the math manageable, we use Voigt Notation, mapping the tensor indices to a 6 x 6 matrix representation:

$$11 \rightarrow 1, \quad 22 \rightarrow 2, \quad 33 \rightarrow 3, \quad 23 \rightarrow 4, \quad 13 \rightarrow 5, \quad 12 \rightarrow 6$$

The relationship becomes a matrix equation: $\sigma_I = C_{IJ}\epsilon_J$

where I, J = 1...6.

General form (triclinic):

$$C = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{pmatrix}$$

- According to Neumann's Principle, the symmetry elements of any physical property of a crystal must include the symmetry elements of the point group of the crystal. As the crystal symmetry increases (from Triclinic to Cubic), the number of independent elastic constants decreases because the symmetry operations force certain components to be zero or equal to each other.

The Tensor Transformation Law

A crystal property is a physical quantity. It does not change just because we rotate our coordinate system. However, the components of the tensor representing that property change according to a specific mathematical rule.

If we rotate a coordinate system from axes $x_i \ to \ x_i'$ using a transformation matrix Q_{ij} (direction cosines), the stiffness tensor components transform as:

$$C'_{ijkl} = \sum_{m=1}^{3}\sum_{n=1}^{3}\sum_{o=1}^{3}\sum_{p=1}^{3} Q_{im}Q_{jn}Q_{ko}Q_{lp}C_{mnop}$$

the material looks identical before and after. Therefore, the coefficients must not change:

$$C'_{ijkl} = C_{ijkl}$$

(A) Triclinic (21 constants)

No symmetry → all 21 symmetric components exist.

(B) **Monoclinic (13 constants)**

(Unique axis = 2 or m : equivalent to a 180° rotation about the z-axis)

$$C = \begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & C_{16} \\ C_{12} & C_{22} & C_{23} & 0 & 0 & C_{26} \\ C_{13} & C_{23} & C_{33} & 0 & 0 & C_{36} \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & 0 & 0 & C_{66} \end{pmatrix}$$

The Transformation Matrix (Q):

$$Q = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$(i.e., x \rightarrow -x, y \rightarrow -y, z \rightarrow z)$.

14 -> 1123

Apply the transformation law:

$$C'_{1123} = \sum_{m,n,o,p} Q_{1m} Q_{1n} Q_{2o} Q_{3p} C_{mnop}$$

Since Q is a diagonal matrix ($Q_{ij} = 0$ if $i \neq j$), the only non-zero term in the massive summation is when m=1, n=1, o=2, p=3:

$$C'_{1123} = Q_{11} Q_{11} Q_{22} Q_{33} C_{1123}$$

Substitute the values from matrix Q:

$$C'_{1123} = (-1) \cdot (-1) \cdot (-1) \cdot (1) \cdot C_{1123}$$

$$C'_{1123} = -C_{1123}$$

Apply Symmetry Condition:

Since the crystal has Monoclinic symmetry, C'_{1123} must equal C_{1123}

$$C_{1123} = -C_{1123}$$

$$2C_{1123} = 0 \Rightarrow \mathbf{C_{1123} = 0}$$

In Voigt notation: $\boldsymbol{C_{14} = 0}$

Similarly, the other zero terms can be proved.

Generalization:

Any term with an odd number of index 3 (the z-axis) will be multiplied by $(-1)^{\mathrm{odd}} = -1$ and vanish.

This eliminates: $C_{14}, C_{15}, C_{24}, C_{25}, C_{34}, C_{35}, C_{46}, C_{56}$

Result: 21 constants reduce to 13.

(C) Orthorhombic (9 constants)

Example: mm2 or 222(three perpendicular 2-folds).

$$C = \begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\ C_{13} & C_{23} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{pmatrix}$$

Q_x=diag(1,−1,−1),Q_y=diag(−1,1,−1),Q_z=diag(−1,−1,1)

Now with these transformation matrices, the following constants gets eliminated:

$$C_{16}, C_{26}, C_{36}, C_{45}$$

(D) <u>Tetragonal (6 constants or 7 constants)</u>

Lower Symmetry

$$C = \begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & C_{16} \\ C_{12} & C_{11} & C_{13} & 0 & 0 & \text{-}C_{16} \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ C_{16} & \text{-}C_{16} & 0 & 0 & 0 & C_{66} \end{pmatrix}$$

Higher Symmetry

$$C = \begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{pmatrix}$$

A Tetragonal crystal has a single 4-fold rotation axis (the z-axis).

The Transformation Matrix (Q):

$$x \rightarrow y, \quad y \rightarrow -x, \quad z \rightarrow z$$

Q = $\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

($Q_{12} = 1, Q_{21} = -1$, $Q_{33} = 1$. All others are zero.)

- $C'_{1111} = \sum Q_{1m} Q_{1n} Q_{1o} Q_{1p} C_{mnop}$

The only non-zero value is $Q_{12} = 1$.Therefore, the only surviving term in the sum is when m,n,o,p are all 2.

$$C'_{1111} = Q_{12} Q_{12} Q_{12} Q_{12} C_{2222}$$

$$C'_{1111} = (1)(1)(1)(1) C_{2222}$$

$$C'_{11} = C_{22}$$

Conclusion: Since the material must be invariant ($C'_{11} = C_{11}$), we get:

$$\mathbf{C_{11} = C_{22}}$$

- $C'_{1133} = \sum Q_{1m} Q_{1n} Q_{3o} Q_{3p} C_{mnop}$

Q_{1m}, Q_{1n}: Non-zero only when indices are 2 ($Q_{12} = 1$).

Q_{3o}, Q_{3p}: Non-zero only when indices are 3 ($Q_{33} = 1$).

$$C'_{1133} = Q_{12}Q_{12}Q_{33}Q_{33}C_{2233}$$

$$C'_{13} = (1)(1)(1)(1)C_{23}C'_{13} = C_{23}$$

Conclusion:

$$\mathbf{C_{13} = C_{23}}$$

- $C'_{1313} = \sum Q_{1m}Q_{3n}Q_{1o}Q_{3p}C_{mnop}$

Row 1 terms ($Q_{1\ldots}$) pick index 2.

Row 3 terms ($Q_{3\ldots}$) pick index 3.

$$C'_{1313} = Q_{12}Q_{33}Q_{12}Q_{33}C_{2323}$$

$$C'_{55} = (1)(1)(1)(1)C_{44}$$

$$C'_{55} = C_{44}$$

Conclusion:

$$\mathbf{C_{44} = C_{55}}$$

For lower symmetry group C_{16} is not zero and makes C_{26} = - C_{16} but in higher symmetry adding a mirror reflection($y \rightarrow -y$) makes C_{16} = 0

$C'_{1112} = -C_{2221} = -C_{26}$ (lower symmetry)

$C'_{1112} = -C_{1112} = -C_{16}$ (higher symmetry)

$$C_{16} = -C_{16} \Rightarrow 2C_{16} = 0 \Rightarrow \mathbf{C_{16} = 0}$$

(E) Trigonal (6 constants or 7 constants):

- Lower Symmetry(7 constants):

These crystals have a 3-fold rotation axis (z)

$$C = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & 0 \\ C_{12} & C_{11} & C_{13} & -C_{14} & -C_{15} & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ C_{14} & -C_{14} & 0 & C_{44} & 0 & -C_{15} \\ C_{15} & -C_{15} & 0 & 0 & C_{44} & C_{14} \\ 0 & 0 & 0 & -C_{15} & C_{14} & C_{11}-C_{12}/2 \end{pmatrix}$$

Independent: $C_{11}, C_{33}, C_{44}, C_{12}, C_{13}, C_{14}, \mathbf{C_{15}}$

Rotation by 120:

Q = $\begin{pmatrix} c & s & 0 \\ -s & c & 0 \\ 0 & 0 & 1 \end{pmatrix}$ where $c = \cos(120) = -\frac{1}{2}, \quad s = \sin(120) = \frac{\sqrt{3}}{2}$

The material already possesses Monoclinic Symmetry (with a 2-fold axis along x).

This pre-eliminates terms like $C_{15}, C_{16}, C_{25}, C_{26}, C_{35}, C_{36}, C_{45}, C_{46}$

- Higher Symmetry(6 constants):

$$C = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & 0 & 0 \\ C_{12} & C_{11} & C_{13} & -C_{14} & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ C_{14} & -C_{14} & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & C_{14} \\ 0 & 0 & 0 & 0 & C_{14} & C_{11}-C_{12}/2 \end{pmatrix}$$

Independent: $C_{11}, C_{33}, C_{44}, C_{12}, C_{13}, C_{14}$

Apply a mirror plane at x=0 (reflection $x \ \to -x$).

Matrix $Q = \text{diag}(-1,1,1)$.

$$C'_{1113} = (-1)(-1)(-1)(1)C_{1113} = -C_{15}$$

Since C' = C, we get $C_{15} = -C_{15} \ \Rightarrow \ C_{15} = 0$.

(F) Hexagonal (5 Independent Constants)

- Can be continued from Trigonal

Example: 6/mmm (hexagonal)

$$C = \begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \dfrac{C_{11} - C_{12}}{2} \end{pmatrix}$$

Independent constants:

$$C_{11}, C_{12}, C_{13}, C_{33}, C_{44}$$

Rotation by 60:

Q = $\begin{pmatrix} \text{c} & \text{s} & 0 \\ \text{-s} & \text{c} & 0 \\ 0 & 0 & 1 \end{pmatrix}$ where $c = \cos(60) \ = \ \frac{1}{2}, \quad s = \sin(60) \ = \ \frac{\sqrt{3}}{2}$

By calculating, $C'_{1123} = C'_{14} = \sum Q_{1i}Q_{1j}Q_{2k}Q_{3l}C_{ijkl}$

We get $C'_{14} = -C'_{14} \Rightarrow C_{14} = 0$

(G) Cubic System (3 Independent Constants)

Applies to: m3m, 432, -43m, etc.

$$C = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}$$

Independent constants:

$$C_{11},\ C_{12},\ C_{44}$$

Applying the rotation of 90 deg about the z axis :

$$Q = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

This gives $\mathbf{C_{13}} = \mathbf{C_{23}}$, $\mathbf{C}_{11} = \mathbf{C}_{22}$, $\mathbf{C}_{44} = \mathbf{C}_{55}$

Applying the 3 fold rotation along the diagonal: $x \rightarrow y \rightarrow z$

This proves $\mathbf{C}_{22} = \mathbf{C}_{33}$, $\mathbf{C_{13}} = \mathbf{C}_{12}$, $\mathbf{C}_{44} = \mathbf{C}_{66}$

Crystal system	**Point groups**	**Independent (C_{ij})**
Triclinic	1, -1	21
Monoclinic	2, m, 2/m	13
Orthorhombic	222, mm2, mmm	9
Tetragonal	4, -4, 4/m; 422, 4mm, -42m, 4/mmm	6 or 7
Trigonal	3, -3; 32, 3m, -3m	6 or 7
Hexagonal	6, -6, 6/m; 622, 6mm, -62m, 6/mmm	5
Cubic	23, m3, 432, -43m, m3m	3